

6-Mercaptopurine
50-44-2 | DTXSID0020810

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 1.35e-01

Global applicability domain: Inside

Local applicability domain index: 4.62e-01

Confidence level: 6.51e-01

Nearest Neighbors from the Training Set

[Image not found](#)

6-Mercaptopurine

Measured: 0.01

Predicted: 1.35e-01

[Image not found](#)

Hypoxanthine

Measured: -1.11

Predicted: -0.583

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1-(5-Nitrothiazol-2-yl)imidazolidine-2-thione

Measured: 1.70

Predicted: 1.12